Tailor-made Design of Chemical Blends using Decomposition-based Computer-aided Approach

Yunus, Nor Alafiza; Manan, Zainuddin Abd.; Gernaey, Krist; Woodley, John; Gani, Rafiqul

Publication date:
2011

Document Version
Publisher's PDF, also known as Version of record

Design of tailor-made chemical blend using a decomposition-based computer-aided approach

Nor Alafiza Yunus[a], Krist V. Gaerney[a], Zainuddin Abdul Manan[b], John M. Woodley[a] and Rafiqul Gani*[a]

[a] Department of Chemical and Biochemical Engineering, Søltofts Plads, Building 229, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark.

[b] Process System Engineering Centre (PROSPECT), Faculty of Chemical and Natural Resources Engineering, UTM Skudai, 81310, Johor Bahru, Johor, Malaysia

Computer aided technique is an efficient approach to solve chemical product design problems such as design of blended liquid products (chemical blending). In chemical blending, one tries to find the best candidate, which satisfies the product targets defined in terms of desired product attributes (properties). In this way, first the systematic computer-aided technique establishes the search space, and then narrows it down in subsequent steps until a small number of feasible and promising candidates remain and then experimental work may be conducted to verify if any or all the candidates satisfy the desired product attributes. Alternatively, rigorous modelling could also be used in this final step. In other words, the candidates are quickly generated and screened until a small number is left for final selection and evaluation by experiment and/or rigorous modelling.

This paper presents a design methodology for blended liquid products that identifies a set of feasible chemical blends. The blend design problem is formulated as a nonlinear programming (NLP) model where the objective is to find the optimal blended gasoline or diesel product subject to blend chemicals and their compositions, a set of desired properties of the product as design constraints. The blend design problem is solved using a decomposition approach, which eliminates infeasible and/or redundant candidates gradually. The decomposition method reduces the search space in a systematic way. This general blend design problem is decomposed into two stages. The first stage investigates the mixture stability where all unstable mixtures are eliminated and the stable blend candidates are retained for further testing. In the second stage, the blend candidates have to satisfy a set of target properties that are ranked according to a specified priority. Finally, a short list of candidates, ordered in terms of specified performance criteria, is produced for final testing and selection. This systematic and computer-aided approach is illustrated through a case study involving the design of blends of gasoline with oxygenates from biomass for use in internal combustion engines. The blend design formulation is able to find the optimal blend candidate.

Keywords: blend; decomposition method; tailor-made chemical

* Corresponding author (Email: rag@kt.dtu.dk, Tel. +45 45252882, Fax: +45 45932906)